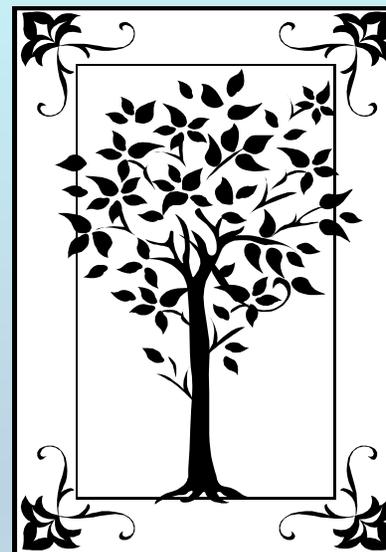


COMPOUND ENTRY tutorial #2

New Compounds

Guided Data Capture (GDC)



This tutorial demonstrates how to add **COMPOUNDS**, which are **NOT** included in the database provided with the Guided Data Capture (GDC) software.

The *GDC* software includes an integrated searchable database of more than 100,000 compounds. Most compounds can be selected from this database.

This tutorial describes how to add new compounds **NOT** included in the GDC compound database.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

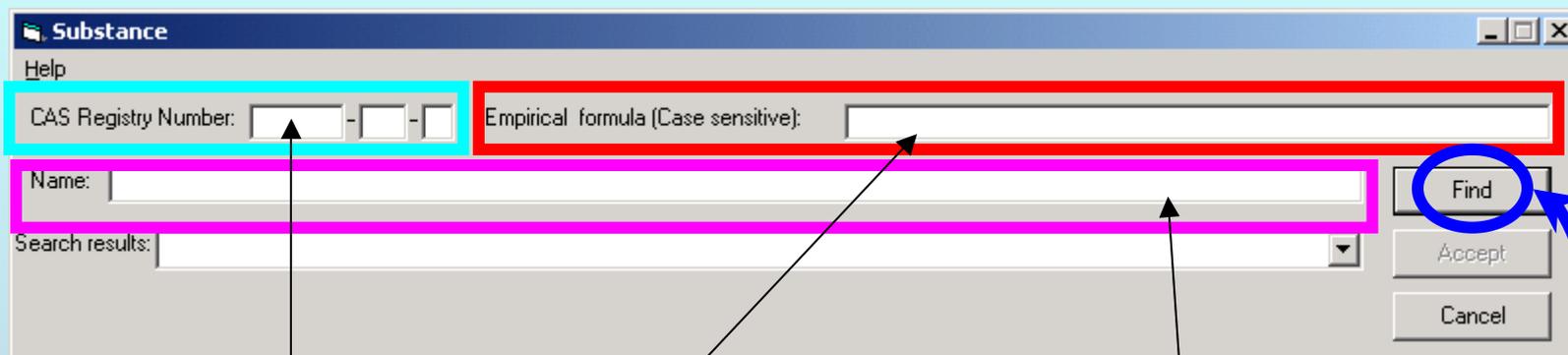
Reference Compound Sample Mixture Reaction Property Data Tables

2002 chi dik 0

**1. SELECT (i.e.,
click once) the
reference code**

**2. CLICK
*Compound***

Search by Name, CASRN, or elemental formula



The screenshot shows a software window titled "Substance" with a "Help" button. It features three input fields: "CAS Registry Number:" (with three separate boxes for digits), "Empirical formula (Case sensitive):", and "Name:". Below these is a "Search results:" field. On the right side, there are three buttons: "Find", "Accept", and "Cancel". A blue circle highlights the "Find" button, and a blue arrow points from it towards the text box below. Three black arrows point from the text box below to the three input fields: one to the CAS Registry Number boxes, one to the Empirical formula field, and one to the Name field.

1. Type the CASRN, Elemental Formula, and/or Name: **(A) Elemental Formula**

Enter the entire elemental formula or use wildcards (*)
(e.g., C₅H₅N, (NH₂)₂CO, C*H₁₀, C₅H₅*, *Cl₃)

or **(B) Name**

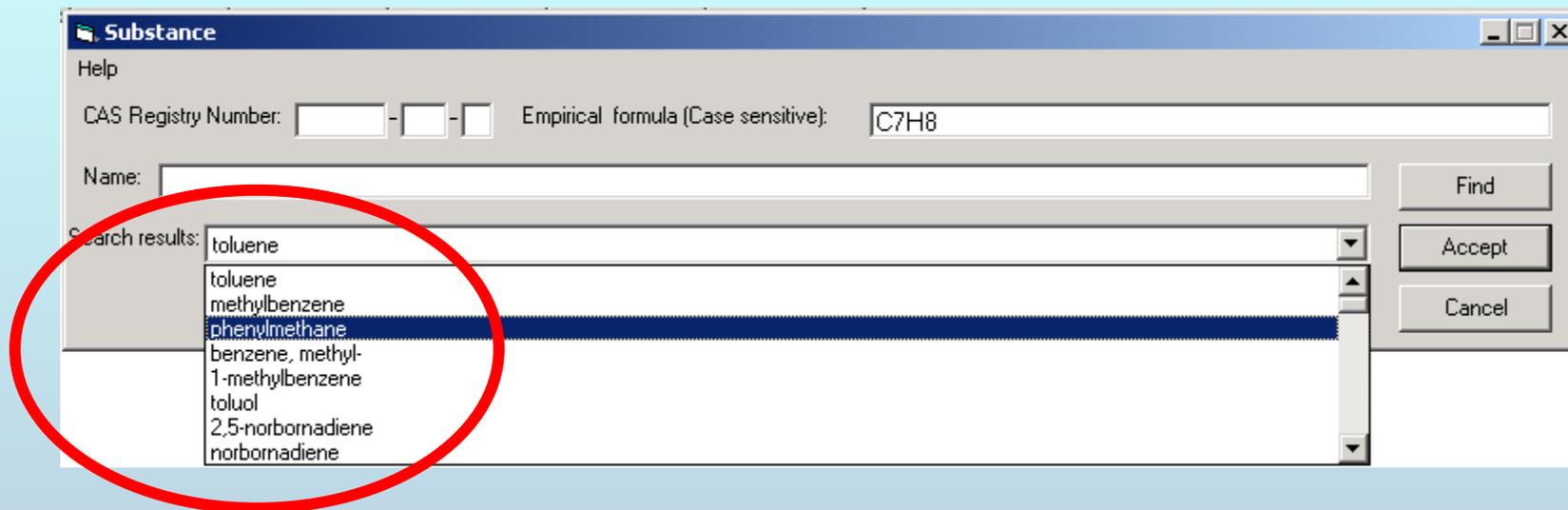
Enter the entire name or use wildcards (*)
(e.g., 2-methylpyridine, 2-methylp*, 2-*pyridine)

or **(C) CASRN**

Enter the CASRN; the final digit is filled automatically.

2. CLICK *Find* to complete the search

If you cannot find your compound in the list:



1. Check to see if the compound is listed under an alternative name (e.g., 2-methylpyridine rather than beta-picoline)

2. Continue with tutorial

NOTE: Numerous synonyms are provided in the GDC compound database, but it is not exhaustive.

The image shows a software dialog box titled "Substance". It contains several input fields and buttons. A red box highlights the "CAS Registry Number" field (with three empty boxes) and the "Name" field (containing "Compound X name"). A blue box highlights the "Accept" button. Red arrows point from the text boxes to the highlighted fields, and a blue arrow points from the text box to the "Accept" button.

Substance

Help

CAS Registry Number: - - Empirical formula (Case sensitive):

Name:

Search results:

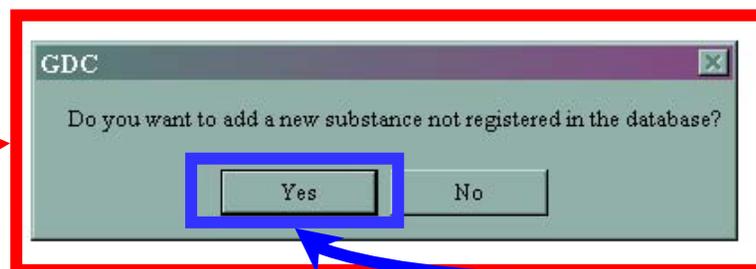
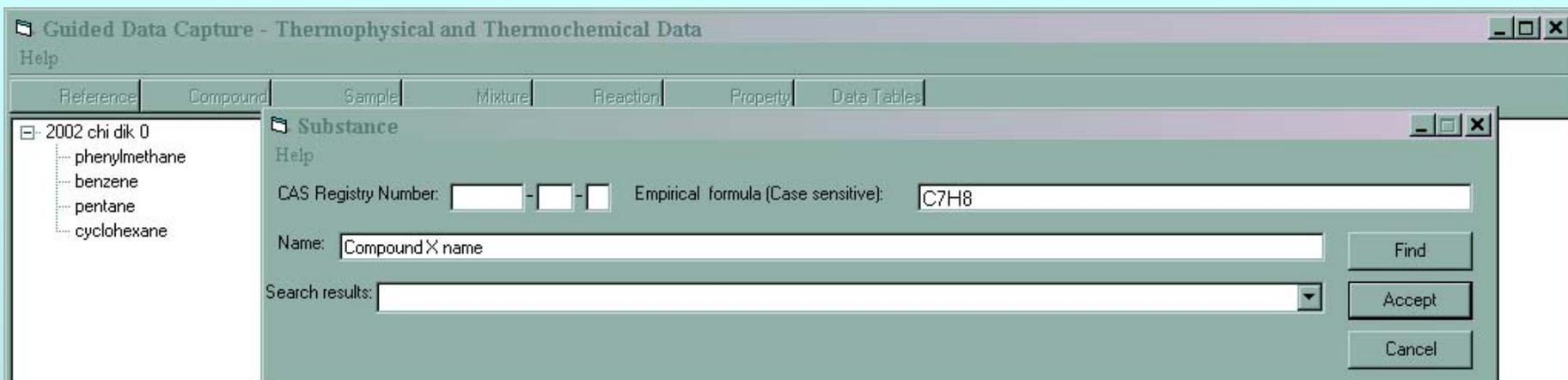
Find

Accept

Cancel

1. TYPE in the new compound name (and CASRN, only if known)

2. CLICK *Accept*



1. This dialog box will appear

2. CLICK *Yes*

NOTE: The GDC program will assign a temporary CASRN, if you do not provide one.

Guided Data Capture - Thermophysical and Thermochemical Data

Help

Reference Compound Sample Mixture Reaction Property Data Tables

2002 chi dik 0

- phenylmethane
- benzene
- pentane
- ...
- Compound X name

Substance

Help

CAS Registry Number: - - Empirical formula (Case sensitive):

Name:

Search results:

Find

Accept

Done

1. The new compound now appears in the program list.

2. Continue adding compounds.

CLICK *Done*, when finished.

Start | Welcome to ... | Guided Data... | N:\TRC Dat... | COMPOUN... | COMPOUN... | Substance | 3:33 PM

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

- 2002 chi dik 1
 - phenylmethane
 - benzene
 - hexane
 - cyclopentane

Any number of compounds can be added.

Start | [Icons] | Eud... | Wel... | Gui... | Gett... | Com... | Cal... | [Icons] | 4:21 PM

END

See the **SAMPLE Entry** tutorial to continue, or use the **HELP** screens provided within the **GDC** program.